«beta»-Alanine, N-(3-fluorobenzoyl)-, hexyl ester

Inchi: InChI=1S/C16H22FNO3/c1-2-3-4-5-11-21-15(19)9-10-18-16(20)13-7-6-8-14(17)12-13/h6

InchiKey: YOYUEPRUTMTMNH-UHFFFAOYSA-N

Formula: C16H22FNO3

SMILES: CCCCCCOC(=O)CCNC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 295.35

Physical Properties

Property code	Value	Unit	Source
gf	-281.64	kJ/mol	Joback Method
hf	-648.53	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.069		Crippen Method
mcvol	233.300	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook
tb	776.74	K	Joback Method
tc	974.77	K	Joback Method
tf	484.36	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.53	J/mol×K	776.74	Joback Method
cpg	698.81	J/mol×K	809.75	Joback Method
cpg	712.15	J/mol×K	842.75	Joback Method
cpg	724.58	J/mol×K	875.76	Joback Method
cpg	736.14	J/mol×K	908.76	Joback Method
cpg	746.84	J/mol×K	941.77	Joback Method
cpg	756.71	J/mol×K	974.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321936&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume